Chapter 1

Introduction

1.1 Fractional Calculus

Derivatives of integer order have been widely known and commonly used since the origin of the Calculus (17^{th} century) however, non-integer order derivatives seem not to be very well known but have been considered since Lebinitz [1]. The first historical application of fractional calculus was discussed by N.H. Abel, commonly known as Abel's tautochrone problem [2]. The study of fractional calculus has been solely related to the field of Mathematics for many years [3]. However, in the recent few years, several physical and chemical phenomena have been modeled by fractional derivatives and integrals due to their vital property of providing mechanism to incorporate the hereditary properties of such phenomena. The non-local behavior of fractional derivatives and integrals makes it effective for modeling some phenomena in nature having memory effects, such as human behavior, business, viscoelasticity, etc. Fractional calculus has a broad range of applications in physics [4], biology [5], control theory [6], bioengineering [7], thermodynamics [8] etc. For further reference and detailed study, we refer to a few textbooks on fractional calculus by Oldham & Spanier [9], Miller & Ross [10], Podlubny [3], and Kilbas [11].

1.2 Preliminaries

In this section, we provide some basic definitions and properties of fractional derivatives and integrals used throughout this thesis. The integrals presented here are assumed to be finite and all the definitions considered are left sided.

1.2.1 Basic Definitions

Definition 1.2.1. Let $[a,b] \subset \mathbb{R}$ be a finite interval and $f \in \mathrm{L}^1[a,b]$. The **Riemann-Liouville fractional integral** of the function f of order $\alpha \in \mathbb{R}^+$ is defined as [11],

$$I_{a^+}^{\alpha} f(t) = \frac{1}{\Gamma(\alpha)} \int_a^t (t-s)^{\alpha-1} f(s) ds, \quad t > a. \tag{1.1}$$

Definition 1.2.2. Let $[a,b] \subset \mathbb{R}$ be a finite interval and $f \in \mathrm{L}^1[a,b]$. The **Riemann-Liouville fractional derivative** of the function f of order $\alpha \in \mathbb{R}^+$, such that $m-1 < \alpha < m$, $m \in \mathbb{N}$ is defined as [11],

$$\begin{aligned} {}_a^{RL}D_t^{\alpha} f(t) &= D^m I_{a^+}^{m-\alpha} f(t) \\ &= \frac{1}{\Gamma(m-\alpha)} \frac{d^m}{dt^m} \int_a^t (t-s)^{m-\alpha-1} f(s) ds, \quad t > a. \end{aligned} \tag{1.2}$$

Definition 1.2.3. Let $[a,b] \subset \mathbb{R}$ be a finite interval, and $f \in \mathrm{AC}^m[a,b]$. The **Caputo fractional derivative** of the function f of order $\alpha \in \mathbb{R}^+$, such that $m-1 < \alpha < m$,

$m \in \mathbb{N}$ is defined as [11],

$$
\begin{aligned}
{}_a^C D_t^\alpha f(t) &= I_{a^+}^{m-\alpha} D^m f(t) \\
&= \frac{1}{\Gamma(m-\alpha)} \int_a^t (t-s)^{m-\alpha-1} f^{(m)}(s) ds, \quad t > a. \qquad (1.3)
\end{aligned}
$$

1.2.2 Prabhakar Fractional Derivatives and Integrals

To define the Prabhakar fractional derivatives and integrals first we need to define the three parameter Mittag-Leffler (ML) function/ Prabhakar function [12].

Definition 1.2.4. For any $z \in \mathbb{C}$, we define the three parameter ML function/ Prabhakar function as,

$$
E_{\alpha,\beta}^{\gamma}(z) = \sum_{m=0}^{\infty} \frac{\Gamma(\gamma+m) z^m}{\Gamma(\gamma)\Gamma(\alpha m+\beta) m!} \qquad (1.4)
$$

where, $\alpha, \beta, \gamma \in \mathbb{C}$ and $\mathrm{Re}(\alpha) > 0$.

- When $\gamma = 1$, it reduces to two parameter ML function as,

$$
\begin{aligned}
E_{\alpha,\beta}^{1}(z) &= \sum_{m=0}^{\infty} \frac{\Gamma(1+m) z^m}{\Gamma(\alpha m+\beta) m!} \\
&= \sum_{m=0}^{\infty} \frac{z^m}{\Gamma(\alpha m+\beta)} \\
&= E_{\alpha,\beta}(z).
\end{aligned}
$$

- When $\gamma = 0$,

$$
E_{\alpha,\beta}^{0}(z) = \frac{1}{\Gamma(\beta)} + \sum_{m=1}^{\infty} \frac{\Gamma(\gamma+m) z^m}{\Gamma(\gamma)\Gamma(\alpha m+\beta) m!} = \frac{1}{\Gamma(\beta)},
$$

as for $m \geq 1$,

$$\frac{\Gamma(\gamma+m)}{\Gamma(\gamma)} = (\gamma+m-1)(\gamma+m-2)\dots\gamma.$$

- **Properties of Prabhakar function:**

- For any $t \in \mathbb{R}^+$ and $\lambda \in \mathbb{C}$,

$$\int_0^t u^{\beta-1} E^{\gamma}_{\alpha,\beta}(\lambda u^{\alpha}) du = t^{\beta} E^{\gamma}_{\alpha,\beta+1}(\lambda t^{\alpha}).$$

- For any $m \in \mathbb{N}$,

$$\frac{d^m}{dt^m}\left[t^{\beta-1} E^{\gamma}_{\alpha,\beta}(\lambda t^{\alpha})\right] = t^{\beta-m-1} E^{\gamma}_{\alpha,\beta-m}(\lambda t^{\alpha}).$$

Definition 1.2.5. [13] Let $f \in \mathrm{L}^1[a,b]$ and $n-1 < \mathrm{Re}(\alpha) < n$, $-\infty < a < x < b < \infty$, then we define **Prabhakar integral** of order α as,

$$I^{\gamma}_{\rho,\alpha,\omega,a} f(x) = \int_a^x (x-s)^{\alpha-1} E^{\gamma}_{\rho,\alpha}(\omega(x-s)^{\rho}) f(s) ds, \tag{1.5}$$

where $\rho, \alpha, \omega, \gamma \in \mathbb{C}$ and $\mathrm{Re}(\rho),\ \mathrm{Re}(\alpha) > 0$.

Definition 1.2.6. [13] For $f \in \mathrm{L}^1[a,b]$ and $n-1 < \mathrm{Re}(\alpha) < n$, we define **Riemann-Liouville Prabhakar derivative** of order α as,

$$\begin{aligned} {}^{\mathrm{RLP}}_{a}D^{\gamma}_{\rho,\alpha,\omega} f(x) &= \frac{d^n}{dt^n} I^{-\gamma}_{\rho,n-\alpha,\omega,a} f(t) \\ &= \frac{d^n}{dt^n} \int_a^t (t-s)^{n-\alpha-1} E^{-\gamma}_{\rho,n-\alpha}(\omega(t-s)^{\rho}) f(s) ds, \end{aligned} \tag{1.6}$$

where $\rho, \alpha, \omega, \gamma \in \mathbb{C}$.

Definition 1.2.7. [13] For $f \in \mathrm{AC}^n[a,b]$ and $n-1 < \mathrm{Re}(\alpha) < n$, we define **Caputo–Prabhakar derivative** of order α as,

$$\begin{aligned} {}^{\mathrm{CP}}_{a}D^{\gamma}_{\rho,\alpha,\omega} f(t) &= I^{-\gamma}_{\rho,n-\alpha,\omega,a} \frac{d^n}{dt^n} f(t) \\ &= \int_a^t (t-s)^{n-\alpha-1} E^{-\gamma}_{\rho,n-\alpha}(\omega(t-s)^{\rho}) f^{(n)}(s) ds, \end{aligned} \tag{1.7}$$

where $\rho, \alpha, \omega, \gamma \in \mathbb{C}$.

1.3 Model Problems

In this section, we have briefly described the model problems studied in this thesis. We will elaborately lay out these model problems at the beginning of the subsequent chapters for clarity of the presentation. The concise description of the model problems considered in this thesis is given below:

1.3.1 Time Fractional Advection–Diffusion Equation

Here, we consider the following time fractional advection–diffusion equation,

$$\begin{cases} {}^{\mathrm{CP}}_{0}D^{\gamma}_{\rho,\alpha,\omega} u(x,t) = K \frac{\partial^2 u(x,t)}{\partial x^2} - V \frac{\partial u(x,t)}{\partial x} + F(x,t), \qquad 0 < x < L,\ 0 < t \le T \\ u(x,0) = u_0(x), \\ u(0,t) = \eta_1(t), \\ u(L,t) = \eta_2(t), \end{cases} \tag{1.8}$$

where $V > 0$, $K > 0$ are the average fluid velocity and diffusion coefficient, respectively. Here $F(x,t)$, $u_0(x)$, $\eta_1(t)$ and $\eta_2(t)$ are sufficiently smooth known functions. The order of the fractional derivative is $0 < \alpha < 1$ and ${}_{0}^{\mathrm{CP}}D^{\gamma}_{\rho,\alpha,\omega}$ is the time fractional Caputo–Prabhakar derivative.

1.3.2 1D Time Fractional Reaction–Diffusion Equation

Consider the following nonlinear time fractional reaction–diffusion equation,

$$\begin{cases} {}_0D_t^{\alpha}u(x,t) = K\frac{\partial^2 u}{\partial x^2} + f(u) + F(x,t), \qquad (x,t) \in \Omega \times (0,T] \\ u(x,0) = u_0(x), \text{ on } \Omega \\ u(a,t) = u_a(t), \\ u(b,t) = u_b(t), \text{ on } [0,T] \end{cases} \tag{1.9}$$

where $\bar{\Omega} = [a,b]$, $K > 0$, is the diffusion coefficient, $f(u)$ is the reaction term which satisfies the Lipschitz condition,

$$|f(u(x_1,t)) - f(u(x_2,t))| \leq L|u(x_1) - u(x_2)|, \forall x_1, x_2 \in \Omega, \tag{1.10}$$

with L as a positive Lipschitz constant and $F(x,t)$, $u_0(x)$, $u_a(t)$, $u_b(t)$ are sufficiently smooth known functions. The fractional exponent $\alpha \in (0,1)$ and the fractional derivative is defined in the Caputo sense and Caputo–Prabhakar sense.

1.3.3 2D Time Fractional Reaction–Diffusion Equation

Consider the two-dimensional nonlinear Caputo time fractional reaction–diffusion equation with Dirichlet boundary condition on a bounded domain,

$$\begin{cases} {}_0^C D_t^{\alpha} u(x,y,t) = \Delta u(x,y,t) + f(u(x,y,t)) + F(x,y,t), & (x,y,t) \in \Omega \times (0,T] \\ u(x,y,0) = \phi_1(x,y), & (x,y) \in \Omega \\ u(x,y,t) = \phi_2(x,y,t), & (x,y) \in \partial\Omega, t \in (0,T] \end{cases} \tag{1.11}$$

where $\Omega = (0,L) \times (0,L) \subset \mathbb{R}^2$, is a bounded and convex polygon in $\mathbb{R}^2$, $\alpha \in (0,1)$, F is the sufficiently smooth known function and $f(u)$ is a nonlinear function known as reaction term such that it satisfies the Lipschitz condition,

$$|f(u(\mathbf{x},t)) - f(u(\mathbf{y},t))| \leq L|u(\mathbf{x},t) - u(\mathbf{y},t)|, \ \mathbf{x}, \mathbf{y} \in \Omega$$

where L is a positive Lipschitz constant.

1.4 Literature Review

PDEs are used to mathematically formulate the physical phenomena such as the propagation of heat or sound, fluid flow, elasticity, electrostatics, electrodynamics, etc. [14]. However, there are several physical phenomena in nature that involve memory effects and can not be modeled by classical PDEs. Due to the non-locality of fractional derivatives, fractional PDEs become prominent in modeling physical phenomena involving memory, such as, anomalous diffusion and non-local interactions etc. Anomalous diffusion equations are widely used in modeling anomalous diffusive systems, fractional random walk, and unification of diffusion and wave propagation phenomena [15, 16, 17, 18, 19]. Many considerable works on the theoretical analysis of fractional PDEs have been carried out, but due to the non-local nature of fractional derivatives, analytical solutions of most fractional PDEs can not be obtained explicitly, so proposing new methods to find the numerical solution of such equations is of practical importance. Further, a brief literature survey demonstrating motivation behind the research work, carried out in this thesis is presented as follows:

In the very early stage of the twentieth century, a new special function known as the ML function was introduced by Swedish mathematician M.G. Mittag-Leffler during his work on summation methods for divergent series. In 1953, P. Humbert et al. gave its two-parameter generalization [20, 21]. Many researchers used this function to model several mathematical and physical phenomena such as K.S. Cole in the electrical conductance of biological systems [22], B. Gross in the dielectric and mechanical relaxation [23, 24, 25], M. Caputo and F. Mainardi on fractional viscoelasticity [26, 27], and many more [28, 29, 30, 31, 32].

The various applications of the ML function and its two-parameter generalization in both Physics and Mathematics led to the generalization of this function beyond two parameters. Tilak Raj Prabhakar [12] an Indian Mathematician, introduced a three-parameter extension of the ML function, also known as the Prabhakar function. He also studied the convolution integral operator using this function as a kernel. The numerical aspect of this function was discussed by R. Garrappa [33]. He also designed a Matlab code for numerical computation of the Prabhakar function, which is the only code till now for computing the Prabhakar function [34]. In 1954, J.H. Barrett [35] solved a linear differential equation of fractional order using the ML function, hence identified the importance of the ML function in fractional calculus.

Recently, using Prabhakar function as a kernel, Prabhakar fractional integral and Prabhakar fractional derivatives were introduced by Kilbas and Garra known as a generalization of Riemann-Liouville and Caputo type fractional integrals and derivatives. There are many real-world applications of Prabhakar fractional derivatives such as generalized Langevin equations [36], fractional Poisson process [37], fractional maxwell model in linear viscoelasticity [38], and many more [39, 40, 41]. Properties and applications of the Prabhakar function have been studied by Garra et al. in [42] with a special attention to the asymptotic behavior of the function in the complex plane and on the negative semi-axis. Mainardi et al. [43] have examined the local integrability and complete monotonicity of the Prabhakar function. Srivastava et al. [44] established some new connections between the ML functions of one, two, and three parameters and expressed the three-parameter ML function as a fractional derivative of the two-parameter ML function. For a more detailed study of the Prabhakar function and derivatives and integrals involving the Prabhakar function, we refer the readers to [45, 13] and the references therein.

Numerical approximation of Caputo–Prabhakar derivatives have been used to find approximate solutions of fractional-order integro-differential equations using different approaches such as Legendre wavelet method [46], Haar wavelet collocation method [47], and Chebyshev polynomials [48]. Derakhshan et al. studied numerical approximation of fractional Sturm–Liouville problems using Caputo–Prabhakar derivatives [39]. Numerous studies have been done on numerical solutions of fractional-order differential equations with Caputo–Prabhakar derivatives. For example, Eshaghi et al. studied a fractional Black–Scholes model [49] and stability and dynamics of neutral and integro differential systems of fractional order [50]. Derakhshan et al. gave a comparison between homotopy perturbation transform and fractional Adams–Bashforth method for the solution of nonlinear fractional differential equations [51], Garrappa et al. studied stability of fractional-order systems with Caputo–Prabhakar derivative [52].

1.4.1 Literature Review on Time Fractional Advection–Diffusion Equation

To describe solute transport in aquifers, the commonly used equation is the advection–diffusion equation. It is derived from the principle of conservation using Fick's law. The advection–diffusion equation describes advection and diffusion of physical quantities like mass, heat, energy, etc., and it also helps in studying more advanced Navier-Stokes equations [53, 54]. It reduces to a fractional advection–diffusion equation by taking one or more partial derivatives of fractional order. The fractional advection–diffusion equation was first proposed by Chaves [55] to investigate the mechanism of super diffusion and with the goal of having a model able to generate the Levy distribution. Advection–diffusion has been used in describing the transfer of heat in a draining film [56], and transfer of water in soils [57]. It is also used to describe dispersion of tracers in porous media [58], dissolved salts in groundwater [59], dissolved material in estuaries and coastal seas [60], contaminant in shallow lakes [61], and pollutants in rivers and streams [62]. It also describes the transport of pollutants in the atmosphere in long-range [63], forced cooling in turbo generators [64], thermal pollution in river systems [65], and flow in porous media [66]. There are various numerical approaches available in the literature for solving time fractional advection–diffusion equation numerically [67, 68, 69, 70, 71, 72, 73, 74, 75, 76] etc., however, papers available in the literature are quite limited which motivates us to study the effective numerical method for the solution of time fractional advection–diffusion equation where the fractional derivative is taken in the Caputo–Prabhakar sense.

1.4.2 Literature Review on Time Fractional Reaction–Diffusion Equation

Traveling wave solutions of nonlinear reaction–diffusion equations are essential in biological applications and the theory of flame propagation. The physical processes of protein trafficking in body cells, the growth of tumor on sphere, and the model of tissue in developmental biology can be modeled by fractional reaction–diffusion equation. It describes many physical, chemical, biological, and ecological processes, such as mesoscale morphological pattern formation can be modeled by fractional Allen-Cahn equation [77]; different mechanism of pattern formation is described by fractional Gray-Scott model [78, 79]; fractional Bloch-Torrey equation is used to model magnetic resonance [80].

Due to wide applications, in recent years, various numerical methods are developed for solving nonlinear fractional reaction–diffusion equations such as Huang [81, 82] solved time fractional Allen-Cahn equation using finite element method, Li [83] discussed error analysis of Galerkin finite element method for solving nonlinear fractional differential equation with nonsmooth solution, Abbaszadeh et al. [84] solved generalized fractional reaction–diffusion equation by applying mixed finite element method in space with a difference scheme of accuracy two in time, Haghi et al. [85] solved two dimensional nonlinear time fractional reaction–diffusion equations of fourth order using compact finite difference operator for space derivative and weighted-shifted Grunwald difference formula for the time derivative, Hajipour et al. [86] solved the variable order time fractional reaction–diffusion equation using compact difference operator for space discretization and applied weighted and shifted Grunwald difference formula for time discretization. Some other methods include finite difference method [87, 88, 89] and spectral method [90, 91, 92, 93] etc. Li et al. [94] solved nonlinear time fractional reaction–diffusion equations by constructing two new two-grid algorithms for space discretization and using classical L1 scheme for temporal discretization. The H^1, L^2, and L^4 error estimates are given for the fully discretized scheme with convergence order $(2-\alpha)$ in time. Since the typical solution of time fractional differential equations has an initial singularity, the direct implication of these methods leads to some possible accuracy loss. To tackle this difficulty of accuracy loss, researchers have proposed some techniques as follows; M. Stynes [95] solved linear fractional reaction–diffusion equations using $L1$-scheme on the graded mesh and obtained the optimal error estimate of the discussed fully discrete scheme. Cao et al. [89] proposed 2nd-order implicit-explicit time stepping schemes for solving nonlinear fractional differential equations with nonsmooth solutions by introducing correction terms. Jin et al. [96] developed correction formulas at the initial steps to recover the desired accuracy of the backward difference convolution quadrature formula.

1.5 Motivation and Objectives of the Thesis

1.5.1 Motivation

Unlike integer order calculus, many definitions of fractional derivatives and integrals are available in the literature. For the past few decades, many theoretical and experimental studies have been conducted to provide precise definition of fractional operators and study their respective applications. Discussing natural phenomena involving memory effects, nonlocal interactions, and anomalous diffusion more efficiently, studying fractional partial differential equations with new derivatives is one of the scopes that has been encountered in this thesis. We have studied the high-order approximation of the recently proposed Caputo–Prabhakar derivative and its application in solving linear and nonlinear diffusion models.

Further, time fractional diffusion models are used to describe complex physical phenomena with non-local and memory-dependent behaviors. High-order discretization methods can provide more accurate numerical solutions, allowing researchers to capture finer details and better understand the underlying physics. In this thesis, we have solved time fractional advection–diffusion equations and time fractional reaction–diffusion equations using high-order discretization methods. Presented methods provide better accuracy as compared to the existing methods available in the literature.

1.5.2 Objectives

In this thesis, we mainly focus on devising numerical methods for solving time fractional advection–diffusion equation and time fractional reaction–diffusion equations in one and two dimensions using finite difference method and study their analysis thoroughly. In summary, the main objectives of this thesis are as follows:

1. To devise high-order numerical methods for approximating Caputo–Prabhakar derivative using time stepping interpolation polynomials.

2. To solve time fractional advection–diffusion equation and time fractional reaction–diffusion equation in Caputo–Prabhakar sense using devised numerical scheme and find high order numerical solution of Caputo time fractional reaction–diffusion equation in one and two dimensions.

3. Study the stability, solvability, and convergence analysis of the discussed scheme.

4. To provide the experimental analysis to support the theoretical findings.

1.6 Outline of the Thesis

This thesis focuses on obtaining the high order numerical solution of linear and non linear time fractional partial differential equations using finite difference method. The rest of the thesis includes six chapters and its outline is given as follows:

In **Chapter 2** the numerical approximation of Caputo–Prabhakar derivative is discussed using two numerical schemes, and the discussed schemes are adopted to solve the time fractional advection–diffusion equation whose time fractional derivative is defined in the Caputo–Prabhakar sense. In the process of developing the numerical schemes, linear and quadratic interpolation polynomials are used. Further, the devised numerical schemes are combined with central difference approximation to solve the time fractional advection–diffusion equation. Convergence order of the whole discretized schemes are $(\tau^{2-\alpha}, h^2)$ and $(\tau^{3-\alpha}, h^2)$ for linear and quadratic approximations, respectively. Stability and solvability of the numerical schemes are discussed. A comparative numerical experimentation of the two schemes is demonstrated to support the theoretical findings.

Chapter 3 is an extension of the chapter 2, where an rth-degree interpolation polynomial is used to approximate the Caputo–Prabhakar derivative. Further, this approximation together with the central difference approximation, is used to numerically solve the linear time fractional advection–diffusion equation and nonlinear time fractional reaction–diffusion equations. It is shown that the fully discretized scheme is stable, uniquely solvable, and convergent with convergence order $(\tau^{r+1-\alpha}, h^2)$. Numerical results are presented to validate the theoretically claimed results.

In **Chapter 4** a high-order numerical scheme is proposed and analyzed to solve the nonlinear Caputo time fractional reaction–diffusion equation. The numerical scheme is developed using a time stepping cubic approximation scheme in the time direction and a compact finite difference scheme in the spatial direction. The nonlinear reaction term is approximated using the Newton-linearized method. The numerical scheme is proved to be uniquely solvable, and stability is discussed using von Neumann analysis. Further, the scheme is proved convergent in the Euclidean norm with convergence order $(\tau^{4-\alpha}, h^4)$. Numerical experiments are performed to demonstrate the authenticity of the proposed scheme.

Chapter 5 deals with the two-dimensional nonlinear Caputo time fractional reaction–diffusion equation. The Caputo derivative is approximated using the $L2-1_\sigma$ scheme on graded mesh, and spatial derivatives are approximated using standard central difference approximation. Further, to reduce the computational cost, the Newton-linearized method and alternating direction implicit scheme are applied. The solvability, stability, and convergence of the devised scheme are studied rigorously. The applicability of the discussed scheme is established by providing two test examples having smooth and nonsmooth solutions.

Finally, **Chapter 6** concludes the thesis and gives a brief summary of the results highlighting the contribution made by this thesis and discusses future scope of the presented research work.

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